Computer Program Abstracts

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UNITCELL: a nonlinear least-squares program for cell-parameter refinement implementing regression and deletion diagnostics

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The crystallographic problem: During the refinement of unit-cell parameters from the observed positions of Bragg reflections in powder diffraction patterns, errors in the indexing and measurement of reflections are usually identified by their associated large residuals (*e.g.* $2\theta_{obs} - 2\theta_{calc}$). A more robust approach to the identification of such outliers in a data set is to employ regression diagnostics (Belsey, Kuh & Welsh, 1980; Powell, 1985; Holland & Redfern, 1997). The program *UNITCELL* refines cell parameters by minimizing residuals in the experimentally determined Bragg position (in terms of $2\theta_{hkl}$, d spacing d_{hkl} or energy E_{hkl}) using a nonlinear least-squares method. Regression diagnostics are provided that give information on the sensitivity of the refinement result to individual reflection positions (the leverage of each datum), as well as deletion diagnostics that indicate how deleterious each observed position is to the overall fit and automatically compute the effect of removing individual potentially deleterious observations from the data set. Hence, outliers may be identified, remedial action taken, and the overall refinement improved upon.

Method of solution: From an indexed list of Bragg positions (in Q_{hkl}, $2\theta_{hkl}$, d_{hkl} or E_{hkl} provided in the input data file), *UNITCELL* refines the unit-cell parameters by first obtaining an initial estimate of the cell parameters from minimization of residuals in Q_{hkl} by linear least squares [given the crystal system and following Kelsey (1964)] and then conducting nonlinear least-squares refinement, minimizing the residuals in the measured (or other user-specified) variable following the approach of Marquardt [as described by Bevington & Robinson (1992)]. This two-step approach therefore requires no initial guess for the cell parameters. The program then computes regression diagnostics for each reflection, determining its Hat (leverage or influence on the calculated parameters), the change in standard error of the residuals obtained by removing it from the data set (how harmful it is to the fit), the magnitude of its residual corrected for leverage, the influence it has on its own calculated position (which is large if it is an outlier), and the change expected in each calculated cell parameter should the reflection be removed from the data set. Used together, these diagnostics are particularly useful in assessing any individual sources of error in a cell-parameter refinement. The user has the option of outputting diagnostics for every datum, or for a limited number of data points that lie beyond statistically defined cut-off values that indicate that they may be either influential or deleterious to the fit.

Software environment: *UNITCELL* will run under both PC Windows and Apple Macintosh system 6 onwards. The Macintosh version was developed using Symantec Think Pascal and the PC Windows version was implemented using Borland's Turbo Pascal for Windows. The Macintosh version is designed to be interactive with a user-friendly graphical user interface. The crystal system, data type (Q_{hkl}, $2\theta_{hkl}$, d_{hkl} or E_{hkl}), wavelength or 2θ angle, quantity to be minimized in the refinement (residuals in Q_{hkl}, $2\theta_{hkl}$, d_{hkl} or E_{hkl}) and input and output files are specified *via* an interactive input screen, with menu options. The PC Windows version is less elaborate, these specifications being incorporated within the first few lines of the input data file.

The output results are displayed in their own text window, as well as being saved to a user-specified output file. The output file for the PC Windows version is plain text; the output file for the Macintosh version can be written in one of seven user-specified editor formats (MS Word, EDIT II, Vantage/McSink, BBEdit, QEDM, Generic Text or TeachText).

Hardware environment: *UNITCELL* will run on any Apple Macintosh with or without FPU (both versions available; PPC users should employ the non-FPU version). The Windows version has been run on PC-compatible computers from 386 upwards. The executable PC Windows version is 80 kbytes. The source code comprises some 1991 lines of Pascal.

Documentation: A README file accompanies the program giving further details of the deletion diagnostics and use of the program. Example input and output files are also provided.

Availability: The executable code is freely availably by anonymous FTP from rock.esc.cam.ac.uk, where it resides in directory pub/minp/UnitCell/, or from the World Wide Web server at the Department of Earth Sciences, Cambridge University (http://www.esc.cam.ac.uk/mineral_sciences/UnitCell.html).

In case of difficulty, contact the authors by e-mail (tjbh@esc.cam.ac.uk or satr@esc.cam.ac.uk) for further help. Requests for the source code should be directed to the first author by e-mail.

Keywords: Unit-cell refinement, nonlinear least squares, regression diagnostics, deletion

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RSD-PLOT: a program for plotting Rietveld refinement data

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The crystallographic problem: The Rietveld method is a widely used tool in powder diffraction structure refinement. Several refinement programs are available, such as *FAT-Rietan* and *DBWS*. Often, however, scientists see themselves confronted with the problem of plotting or viewing the data. Some utilities to that purpose are available, but these are often commercial or shareware programs that cannot be distributed freely. *RSD-PLOT* was primarily designed as a suite for F. Izumi's *FAT-Rietan* (Young, 1995). It also reads *DBWS* data files and in future the import possibilities will be extended to other formats, such as *GSAS* data files. *RSD-PLOT* is freeware.